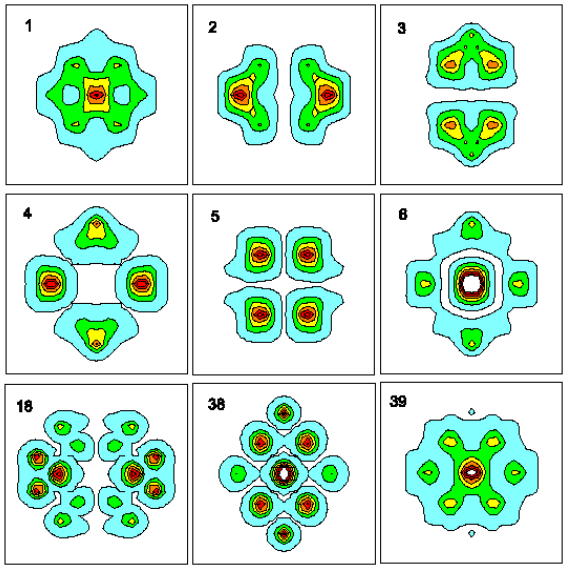
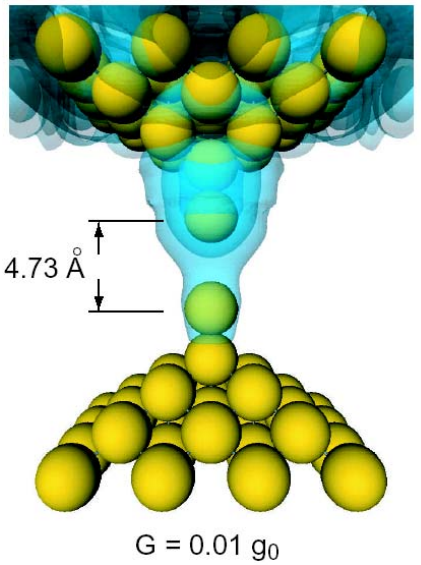
ITR: Modeling and Simulations of Quantum Phenomena in Semiconductor Structures of Reduced Dimensions

Mei-Yin Chou and Uzi Landman (Georgia Tech), Cyrus Umrigar (Cornell University), Xiao-Qian Wang (Clark Atlanta University); DMR-0205328

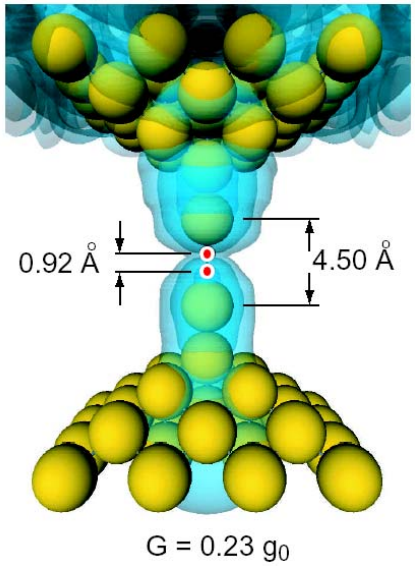
We are conducting a comprehensive simulation of the electrical, optical, structural, and transport properties of various nanowires, with the focus on their size dependence. The goal is to make use of the computational capabilities provided by today's information technology to perform theoretical modeling of materials that may play a key role in the hardware development for tomorrow's information technology. Issues being examined include stability and growth, electronic structure, vibrational modes, conductance, and nanocontacts.



Band-by-band charge distribution in Si nanowire



Insulating broken nanowire



Conducting H_2-welded nanowire

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Education and Outreach

- Train students (undergraduate and graduate) and postdocs in computational techniques for materials simulations
- Involve undergraduate students in materials research through the existing REU program at Georgia Tech
- Partnership between Georgia Tech and Clark Atlanta University (a Historically Black University): co-advising Ph.D. students; regular exchange visits of faculty and students; joint seminars; joint courses; joint workshops
- Minority students in the project: Alexis Nduwimana (Georgia Tech), Damian Cupid (Clark Atlanta), Anthony Cochran (Clark Atlanta), Carmen Robinson (Clark Atlanta), Robert Easley, Jr. (Clark Atlanta)

2003 Activities

- Information Technology Research Seminars
- Mini-workshop on Quantum Approximate Methods for Novel Materials (Clark Atlanta University, October 2003); all participants are minority students
- Special course “Physics of Small Systems” taught by Landman